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LOGINID: ssptansc1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * * * * * *
                     Welcome to STN International
                                                   * * * * * * * * * *
NEWS
                 Web Page for STN Seminar Schedule - N. America
NEWS 2 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN
NEWS 8 DEC 14 BEILSTEIN pricing structure to change
NEWS 9 DEC 17 USPATOLD added to additional database clusters
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
                 MEDLINE segment
NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14 DEC 17 CA/CAplus enhanced with new custom IPC display formats
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
                 from USPATOLD
NEWS 16 JAN 02
                 STN pricing information for 2008 now available
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
                 prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
                 custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
                 of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                 U.S. National Patent Classification
NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
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NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
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FILE 'HOME' ENTERED AT 18:40:05 ON 07 MAR 2008

=> fil reg
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.21
0.21

FILE 'REGISTRY' ENTERED AT 18:40:17 ON 07 MAR 2008
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STRUCTURE FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1 DICTIONARY FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10579564.str

chain nodes :
7 14 15 16
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 13 20 21 22 23
chain bonds :
5-7 7-8 14-15 14-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 10-20 11-12 11-23 20-21
21-22 22-23
exact/norm bonds :
5-7 7-8 8-9 8-12 9-10 11-12 14-15 14-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-20 11-23 20-21 21-22 22-23

G1:[*1],[*2]

G2:0,S

Match level:

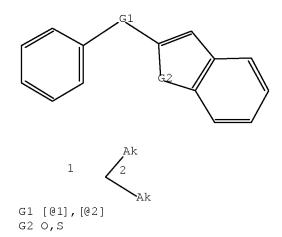
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 20:Atom 21:Atom 22:Atom 23:Atom

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s sss sam 11 SAMPLE SEARCH INITIATED 18:40:59 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 5129 TO ITERATE

39.0% PROCESSED 2000 ITERATIONS

3 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 98286 TO 106874 PROJECTED ANSWERS: 3 TO 319

L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Propanedioic acid, compd. with 2-(2-benzofuranyl)-N-butyl-2-(4-

chlorophenyl)-1,3-dioxolane-4-methanamine (9CI)

MF C22 H24 C1 N O3 . \times C3 H4 O4

CM 1

CM 2

HO2C-CH2-CO2H

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Pyrrolidine, 1-[[2-(2-benzofuranyl)-2-phenyl-1,3-dioxolan-4-yl]methyl]-

MF C22 H23 N O3

```
L2 3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Benzofuran, 2-[4-(bromomethyl)-2-phenyl-1,3-dioxolan-2-yl]-, cis- (9CI)
MF C18 H15 Br O3
```

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

Uploading C:\Program Files\Stnexp\Queries\10579564A.str

```
chain nodes :
7  14  15  16
ring nodes :
1  2  3  4  5  6  8  9  10  11  12  13  20  21  22  23
ring/chain nodes :
25  26
chain bonds :
5-7  7-8  13-25  13-26  14-15  14-16
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  8-9  8-12  9-10  10-11  10-20  11-12  11-23  20-21
21-22  22-23
exact/norm bonds :
5-7  7-8  8-9  8-12  9-10  11-12  13-25  13-26  14-15  14-16
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  10-11  10-20  11-23  20-21  21-22  22-23
```

G1:[*1],[*2]

G2:0,S

Match level :

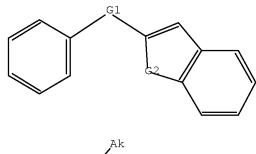
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 25:CLASS 26:CLASS

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



 $\frac{1}{2}$

G1 [@1],[@2] G2 O,S

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

=> s sss sam 13

SAMPLE SEARCH INITIATED 18:44:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5129 TO ITERATE

39.0% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 98286 TO 106874 PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s sss full 13

FULL SEARCH INITIATED 18:48:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 99103 TO ITERATE

100.0% PROCESSED 99103 ITERATIONS

SEARCH TIME: 00.00.03

L5 107 SEA SSS FUL L3

=> save 15 LU10579564/A ANSWER SET L5 HAS BEEN SAVED AS 'LU10579564/A'

=> d scan

L5 107 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 3-Pentanol, 3-[[4-[1-ethyl-1-(6-methoxybenzo[b]thien-2-yl)propyl]-2methylphenoxy]methyl]-

107 ANSWERS

MF C27 H36 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 107 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]-

MF C30 H39 N O5 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 107 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Benzo[b]thiophene-5-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-

MF C27 H34 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

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```
chain nodes :
7 14 15 16
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 13 20 21 22 23
ring/chain nodes :
24 25
chain bonds :
5-7 7-8 13-24 13-25 14-15 14-16
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 8-9 \quad 8-12 \quad 9-10 \quad 10-11 \quad 10-20 \quad 11-12 \quad 11-23 \quad 20-21
21-22 22-23
exact/norm bonds :
5-7 7-8 8-9 8-12 9-10 11-12 14-15 14-16
exact bonds :
13-24 13-25
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 10-11 \quad 10-20 \quad 11-23 \quad 20-21 \quad 21-22 \quad 22-23
```

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 20:Atom 21:Atom 22:Atom

23:Atom 24:CLASS 25:CLASS

L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR

G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> s sss 16 subset=15 sam

SAMPLE SUBSET SEARCH INITIATED 18:51:42 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 0 TO 0 PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L7 0 SEA SUB=L5 SSS SAM L6

=> s sss 16 subset=15 full

FULL SUBSET SEARCH INITIATED 18:51:50 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 38 TO ITERATE

100.0% PROCESSED 38 ITERATIONS 38 ANSWERS

SEARCH TIME: 00.00.01

L8 38 SEA SUB=L5 SSS FUL L6

=> d scan

L8 38 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Methanesulfonic acid, trifluoro-, 2-[1-ethyl-1-[4-(2-ethyl-2-

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 15 not 18

L9 69 L5 NOT L8

=> d scan

L9 69 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, methyl ester

MF C28 H36 O5

$$\begin{array}{c} \text{Me} \\ \text{O} \\ \text{C} \\ \text{D} \\ \text{Et} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil caplus

COST IN U.S. DOLLARS SINCE FILE

ENTRY SESSION

TOTAL

FULL ESTIMATED COST 230.12 230.33

FILE 'CAPLUS' ENTERED AT 18:53:23 ON 07 MAR 2008
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=> s 18

L10 1 L8

=> d ibib abs hitstr

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:493602 CAPLUS $\underline{\text{Full-text}}$

DOCUMENT NUMBER: 143:43764

TITLE: Preparation of substituted benzothiophenes as vitamin

D receptor modulators

INVENTOR(S): Lu, Jianliang; Ma, Tainwei; Nagpal, Sunil; Shen,

Quanrong; Warshawsky, Alan M.; Yee, Ying Kwong; Rupp,

Michael John

PATENT ASSIGNEE(S): Eli Lilly and Company, USA SOURCE: PCT Int. Appl., 308 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND		DATE			APPL	ICAT	DATE							
=					A2		20050609		WO 2004-US37181							20041116			
WO	W: AE, AG, A							DΛ	DD	DC.	DD	D TaT	DV	D7	C_{Λ}	СП			
	VV •																		
		•			•		DE,	•		•				•	•				
							ID,										•		
							LV,												
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
		ТJ,	TM,	TN,	TR,	TT,	ΤZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
		EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LU,	MC,	NL,	PL,	PT,	RO,		
		SE,	SI,	SK,	TR.	BF.	ВJ,	CF.	CG.	CI,	CM,	GA,	GN.	GO,	GW.	ML,	MR,		
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, ,			,	,	A1	20050609			CA 2004-2544522						20041116				
EP 1687292				A2	20060809			EP 2004-819516											
EP									21 2001 019010						2	0041	110		
EE		-							CD	CD	T TT	т т	т тт	NIT	C E	MC	DT		
	K:						ES,								SE,	MC,	PI,		
										CZ, EE, HU, PL, SK, IS						0001111			
-	JP 2007512329				_		2007			JP 2006-541233									
AT 370941					Τ		2007	0915	AT 2004-819516					20041116					

OTHER SOURCE(S): MARPAT 143:43764

GΙ

$$\mathbb{Z}^2$$
 \mathbb{M} \mathbb{Z}^2 \mathbb{M} \mathbb{Z}^3 \mathbb{R}^4 $\mathbb{R}^$

Title compds. I [R, R' = alkyl, fluoroalkyl, etc.; R5, R2 = H, halo, alkyl, fluoroalkyl, etc.; R4, R3, R1 = H, halo, alkyl, fluoroalkyl, etc.; X, Y, M = divalent linking groups; Z2 = branched alkyl, 3-methyl-3-hydroxypentyl, etc.; Z1 = alk(en)yloxy, cycloalkoxy, etc.] are prepared For instance, II is prepared in 5 steps from 2-fluoro-4-iodo-3- trimethylsilanylbenzaldehyde, mercaptoacetic acid, ethylmagnesium bromide, 3-pentanone, o-cresol and 1-bromopinacolone. II has an EC50 = 234 nM in a vitamin D receptor assay. I are less hypercalcemic than $1\alpha,25$ -dihydroxy vitamin D3 and are useful for the treatment of bone disease and psoriasis.

ΙI

IT 853600-60-9P 853600-62-1P 853600-70-1P 853600-72-3P 853600-75-6P 853600-80-3P 853600-82-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted benzothiophenes as vitamin D receptor modulators)

RN 853600-60-9 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 853600-62-1 CAPLUS

CN Benzo[b]thiophene-6-carboxamide, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-N,N-dimethyl- (CA INDEX NAME)

RN 853600-70-1 CAPLUS

CN Benzo[b]thiophene-5-carboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

RN 853600-72-3 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]benzo[b]thien-5-yl]carbonyl]- (CA INDEX NAME)

RN 853600-75-6 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853600-80-3 CAPLUS

CN D-Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & \\ & &$$

RN 853600-82-5 CAPLUS

CN L-Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

IT 853600-61-0P 853600-63-2P 853600-64-3P 853600-65-4P 853600-71-2P 853600-73-4P 853600-74-5P 853600-77-8P 853600-78-9P 853600-79-0P 853600-81-4P 853600-83-6P

853600-84-7P 853600-85-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted benzothiophenes as vitamin ${\tt D}$ receptor modulators)

RN 853600-61-0 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853600-63-2 CAPLUS

CN Benzo[b]thiophene-6-carboxamide, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-N,N-dimethyl- (CA INDEX NAME)

RN 853600-64-3 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]benzo[b]thien-6-yl]carbonyl]- (CA INDEX NAME)

RN 853600-65-4 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]- (CA INDEX NAME)

RN 853600-71-2 CAPLUS

CN Benzo[b]thiophene-5-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853600-73-4 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]benzo[b]thien-5-yl]carbonyl]- (CA INDEX NAME)

RN 853600-74-5 CAPLUS

CN Benzo[b]thiophene-5-carboxamide, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-N,N-dimethyl- (CA INDEX NAME)

RN 853600-77-8 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-[(methylsulfonyl)oxy]benzo[b]thien-2-yl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853600-78-9 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, (+)- (CA INDEX NAME)

Rotation (+).

RN 853600-79-0 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, (-)- (CA INDEX NAME)

Rotation (-).

RN 853600-81-4 CAPLUS

CN D-Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853600-83-6 CAPLUS

CN L-Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853600-84-7 CAPLUS

CN Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]-2-methyl-, methyl ester (CA INDEX NAME)

RN 853600-85-8 CAPLUS

CN Alanine, N-[[2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thien-6-yl]carbonyl]-2-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO2C} \\ \text{Me} \end{array} \\ \text{NH} \\ \text{C} \\ \text{S} \\ \text{Et} \\ \end{array} \\ \begin{array}{c} \text{OH} \\ \text{O-CH}_2 \\ \text{Et} \\ \end{array} \\ \begin{array}{c} \text{OH} \\ \text{Et} \\ \end{array}$$

IT 853601-14-6P 853601-20-4P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of substituted benzothiophenes as vitamin D receptor modulators)

RN 853601-14-6 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+).

RN 853601-20-4 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-).

IT 853601-15-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of substituted benzothiophenes as vitamin D receptor
 modulators)

RN 853601-15-7 CAPLUS

CN Phenol, 4-[1-ethyl-1-(6-methoxybenzo[b]thien-2-yl)propyl]-2-methyl- (CA INDEX NAME)

IT 853600-91-6P 853600-92-7P 853600-93-8P 853601-03-3P 853601-05-5P 853601-06-6P 853601-07-7P 853601-08-8P 853601-09-9P 853601-10-2P 853601-11-3P 853601-12-4P 853601-13-5P 853601-16-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted benzothiophenes as vitamin ${\tt D}$ receptor modulators)

RN 853600-91-6 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-(4-hydroxy-3-methylphenyl)propyl]- (CA INDEX NAME)

RN 853600-92-7 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-(4-hydroxy-3-methylphenyl)propyl]-, methyl ester (CA INDEX NAME)

RN 853600-93-8 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 853601-03-3 CAPLUS

CN Phenol, 4-[1-ethyl-1-(5-methoxybenzo[b]thien-2-yl)propyl]-2-methyl- (CA INDEX NAME)

RN 853601-05-5 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-(5-methoxybenzo[b]thien-2-yl)propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853601-06-6 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-(5-hydroxybenzo[b]thien-2-yl)propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853601-07-7 CAPLUS

CN Methanesulfonic acid, trifluoro-, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]benzo[b]thiophene-5-yl ester (9CI) (CA INDEX NAME)

$$F_{3}C = \begin{bmatrix} & & & & \\$$

RN 853601-08-8 CAPLUS

CN Benzo[b]thiophene-5-carboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

RN 853601-09-9 CAPLUS

CN 3-Pentanol, 3-[[4-[1-ethyl-1-(6-methoxybenzo[b]thien-2-yl)propyl]-2-methylphenoxy]methyl]- (CA INDEX NAME)

RN

CN Benzo[b]thiophene-6-ol, 2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853601-11-3 CAPLUS

CN Methanesulfonic acid, trifluoro-, 2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]benzo[b]thiophene-6-yl ester (9CI) (CA INDEX NAME)

$$F3C - S - O - CH_2 - C - Et$$

$$Et - C - Et$$

$$Et - C - Et$$

RN 853601-12-4 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-ethyl-2-hydroxybutoxy)-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

RN 853601-13-5 CAPLUS

CN Benzo[b]thiophene-6-carboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-C} \\ \\ \text{MeO-C} \\ \\ \text{Et} \\ \end{array}$$

RN 853601-16-8 CAPLUS

CN Acetic acid, [4-[1-ethyl-1-(6-methoxybenzo[b]thien-2-yl)propyl]-2-

=> s 19 L11 5 L9

=> d ibib abs hitstr 1-5

L11 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:216966 CAPLUS Full-text

DOCUMENT NUMBER: 144:270168

TITLE: Regulating PAS domain function with foreign PAS

ligands

INVENTOR(S): Gardner, Kevin H.; Amezcua, Carlos A.; Erbel, Paulus

J. A.; Card, Paul B.; Harper, Shannon; Rutter, Jared;

Bruick, Richard; McKnight, Steven L.

PATENT ASSIGNEE(S): Board of Regents, The University of Texas System, USA

SOURCE: U.S. Pat. Appl. Publ., 18 pp., Cont.-in-part of U.S.

Ser. No. 677,734.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006051829	A1	20060309	US 2005-245742	20051011
US 6319679	B1	20011120	US 2001-770170	20010126
US 2003059917	A1	20030327	US 2001-59962	20011119
US 7132278	В2	20061107		
US 2005074846	A1	20050407	US 2003-677734	20031001
PRIORITY APPLN. INFO.:			US 2001-770170	A3 20010126
			US 2001-59962	A1 20011119
			US 2003-677734	A2 20031001

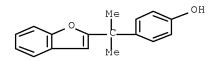
AB A functional surface binding specificity of a PAS domain, wherein the PAS domain is predetd., prefolded in its native state, and comprises a hydrophobic core that has no NMR-apparent a priori formed ligand cavity, is changed by (a) introducing into the hydrophobic core of the PAS domain a foreign ligand of the PAS domain; and (b) detecting a change in the functional surface binding specificity of the PAS domain. The PAS domain is part of PAS kinase.

IT 877820-07-0

RL: BSU (Biological study, unclassified); CST (Combinatorial study, unclassified); BIOL (Biological study); CMBI (Combinatorial study) (regulating PAS domain function with foreign PAS ligands)

RN 877820-07-0 CAPLUS

CN Phenol, 4-[1-(2-benzofuranyl)-1-methylethyl]- (CA INDEX NAME)



L11 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:490363 CAPLUS Full-text

DOCUMENT NUMBER: 143:43763

TITLE: Preparation of substituted benzofuran vitamin d

receptor modulators

INVENTOR(S): Lu, Jianliang; Ma, Tianwei; Nagpal, Sunil; Shen,

Quanrong; Warshawsky, Alan M.; Ochoada, Jason Matthew;

Yee, Ying Kwong

PATENT ASSIGNEE(S): Eli Lilly and Company, USA SOURCE: PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA.	PATENT NO.						KIND DATE				ICAT	ION I	DATE				
WO	WO 2005051938					A1 20050609				 WO 2	004-	US35	20041116				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ŢJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
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	EP 1687289																
		AT,															
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JP	2007		•	•		•		,	•	,					2	0041	116
						T 20070517			US 2006-579563								
	IORITY APPLN. INFO.:					20070310			US 2003-523905P								
									WO 2004-US35529								
OTHER SO	HER SOURCE(S):						143:	43763		2	001		020	,		0041	110

OTHER SOURCE(S): MARPAT 143:43763

GΙ

Title compds. I [R, R' = alkyl, fluoroalkyl, etc.; Rp3, Rb = H, halo, alkyl, etc.; Rp, RF3, Rb' = H, halo alkyl, fluoroalkyl, etc.; Lp1, Lp2, Lfb = divalent linking groups; Zp = alkyl, 3-methyl-3-hydroxypentyl, etc.; Zfb = alkoxy, alkenyloxy, cycloalkoxy, etc.] are prepared For instance, II is prepared in 5 steps from 5-bromo-2-hydroxybenzaldehyde, bromoacetate, ethylmagnesium bromide, o-cresol and 1-bromopinacolone. In an osteocalcin promotor assay (marker for osteoporosis), II has EC50 = 1 nM. I are exhibit vitamin D receptor (VDR) modulating activity that are less hypercalcemic than $1\alpha,25$ -dihydroxy vitamin D3 and are useful for treating bone disease and psoriasis.

IT 853598-34-2P 853598-36-4P 853598-38-6P 853598-39-7P 853598-42-2P 853598-43-3P 853598-44-4P 853598-46-6P 853598-49-9P 853598-50-2P 853598-71-7P 853598-85-3P 853598-86-4P 853598-87-5P 853598-88-6P 853598-89-7P 853598-90-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted benzofuran vitamin d receptor modulators) 853598-34-2 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN

RN 853598-38-6 CAPLUS

CN 5-Benzofurancarboxamide, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-N,N-dimethyl- (CA INDEX NAME)

RN 853598-39-7 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]- (CA INDEX NAME)

RN 853598-42-2 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

RN 853598-43-3 CAPLUS

CN Alanine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]-2-methyl- (CA INDEX NAME)

RN 853598-44-4 CAPLUS

CN 5-Benzofurancarboxamide, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

RN 853598-46-6 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-[[2-(1,1-dimethylethyl)-1,3-dioxolan-2-yl]methoxy]-3-methylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

RN 853598-49-9 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-(1-methylethyl)phenyl]-1-ethylpropyl]- (CA INDEX NAME)

RN 853598-50-2 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O-CH}_2-\text{C-Bu-t} \\ & \text{Et} & \text{Et} & \text{O-CH}_2-\text{C-Bu-t} \end{array}$$

RN 853598-71-7 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[6-[(methylsulfonyl)oxy]-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853598-85-3 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-86-4 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-87-5 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-88-6 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-89-7 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-(1-methylethyl)phenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]- (CA INDEX NAME)

RN 853598-90-0 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-ethylphenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Et} & \text{O-CH}_2\text{--}\text{C-Bu-t} \\ \text{HO}_2\text{C--}\text{CH}_2\text{--}\text{N--C} & \text{Et} & \text{O-CH}_2\text{--}\text{C--Bu-t} \\ \text{Me} & \text{O} & \text{O-CH}_2\text{--}\text{N--C} & \text{O-CH}_2\text{--C--Bu-t} \\ \end{array}$$

IT 853598-35-3P 853598-37-5P 853598-40-0P

853598-45-5P 853598-47-7P 853598-48-8P

853598-51-3P 853598-52-4P 853598-72-8P

853598-73-9P 853598-74-0P 853598-80-8P

853598-81-9P 853598-94-4P 853598-95-5P

853598-96-6P 853598-97-7P 853598-98-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted benzofuran vitamin d receptor modulators)

RN 853598-35-3 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

RN 853598-37-5 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853598-40-0 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-5-benzofuranyl]carbonyl]- (CA INDEX NAME)

RN 853598-45-5 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-ethylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

RN 853598-47-7 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-[[2-(1,1-dimethylethyl)-1,3-dioxolan-2-yl]methoxy]-3-methylphenyl]-1-ethylpropyl]- (CA INDEX NAME)

RN 853598-48-8 CAPLUS

CN Glycine, N-[[2-[1-[4-[[2-(1,1-dimethylethyl)-1,3-dioxolan-2-yl]methoxy]-3-methylphenyl]-1-ethylpropyl]-5-benzofuranyl]carbonyl]- (CA INDEX NAME)

RN 853598-51-3 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]- (CA INDEX NAME)

RN 853598-52-4 CAPLUS

CN Glycine, N-[[2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-6-benzofuranyl]carbonyl]- (CA INDEX NAME)

RN 853598-72-8 CAPLUS

CN 6-Benzofuranol, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, 6-(methanesulfonate) (9CI) (CA INDEX NAME)

RN 853598-73-9 CAPLUS

CN Alanine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-5-benzofuranyl]carbonyl]-2-methyl- (CA INDEX NAME)

RN 853598-74-0 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

RN 853598-80-8 CAPLUS

CN 5-Benzofuranol, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, 5-(methanesulfonate) (9CI) (CA INDEX NAME)

RN 853598-81-9 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-[(methylsulfonyl)methyl]-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853598-94-4 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[3-ethyl-4-(2-hydroxy-3,3-dimethylbutoxy)phenyl]propyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

RN 853598-95-5 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-6-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-96-6 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-6-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 853598-97-7 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

853598-98-8 CAPLUS RN

Glycine, N-[[2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-CN methylphenyl]propyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.

853599-80-1 853599-82-3 853599-84-5 ΤT 853599-85-6 853599-88-9 853599-89-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of substituted benzofuran vitamin d receptor modulators) 853599-80-1 CAPLUS

CN Alanine, N-[[2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3methylphenyl]propyl]-5-benzofuranyl]carbonyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

853599-82-3 CAPLUS RN

5-Benzofuranol, 2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3methylphenyl]propyl]-, 5-(methanesulfonate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 853599-84-5 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-(1-methylethyl)phenyl]propyl]-5-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

RN 853599-85-6 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-6-benzofuranyl]carbonyl]-N-methyl- (CA INDEX NAME)

RN 853599-88-9 CAPLUS

CN 5-Benzofurancarboxamide, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-N,N-dimethyl- (CA INDEX NAME)

RN

CN 5-Benzofurancarboxamide, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 853599-63-0 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 853599-64-1 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2S)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted benzofuran vitamin d receptor modulators) 853599-17-4 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-(4-hydroxy-3-methylphenyl)propyl]-, methyl ester (CA INDEX NAME)

RN 853599-18-5 CAPLUS

RN

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-(3-ethyl-4-hydroxyphenyl)propyl]-, methyl ester (CA INDEX NAME)

RN 853599-19-6 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-ethylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

RN 853599-20-9 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-hydroxy-3-(1-methylethyl)phenyl]propyl]-, methyl ester (CA INDEX NAME)

RN 853599-21-0 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-(1-methylethyl)phenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

RN 853599-23-2 CAPLUS

CN Phenol, 4-[1-ethyl-1-[6-(phenylmethoxy)-2-benzofuranyl]propyl]-2-methyl-(CA INDEX NAME)

RN

RN 853599-25-4 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-(6-hydroxy-2-benzofuranyl)propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853599-26-5 CAPLUS

CN Methanesulfonic acid, trifluoro-, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-6-benzofuranyl ester (9CI) (CA INDEX NAME)

RN 853599-27-6 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-[4-(3,3-dimethyl-2-oxobutoxy)-3-methylphenyl]-1-ethylpropyl]-, methyl ester (CA INDEX NAME)

RN 853599-47-0 CAPLUS

CN Phenol, 4-[1-ethyl-1-[5-(phenylmethoxy)-2-benzofuranyl]propyl]-2-methyl-(CA INDEX NAME)

RN 853599-48-1 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-(phenylmethoxy)-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2 - \text{C-Bu-t} \\ \text{Ph-CH}_2 - \text{O-CH}_2 - \text{C-Bu-t} \end{array}$$

RN 853599-49-2 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-(5-hydroxy-2-benzofuranyl)propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2 - \text{C-Bu-t} \\ \\ \text{Et} \end{array}$$

RN 853599-50-5 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-[(methylsulfonyl)oxy]-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853599-52-7 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-(hydroxymethyl)-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853599-53-8 CAPLUS

CN 2-Butanone, 1-[4-[1-ethyl-1-[5-[(methylthio)methyl]-2-benzofuranyl]propyl]-2-methylphenoxy]-3,3-dimethyl- (CA INDEX NAME)

RN 853599-60-7 CAPLUS

CN 5-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-[(2R)-2-hydroxy-3,3-dimethylbutoxy]-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 853599-62-9 CAPLUS

CN 6-Benzofurancarboxylic acid, 2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2 \\ \text{CH-Bu-t} \\ \end{array}$$

RN 853599-66-3 CAPLUS

CN Glycine, N-[[2-[1-ethyl-1-[4-(2-hydroxy-3,3-dimethylbutoxy)-3-methylphenyl]propyl]-6-benzofuranyl]carbonyl]-N-methyl-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1987:439794 CAPLUS Full-text

DOCUMENT NUMBER: 107:39794

TITLE: Preparation of hypoglycemic 2,4-thiazolidinediones INVENTOR(S): Eggler, James F.; Holland, Gerald F.; Johnson, Michael

Ross; Volkmann, Robert A.

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: PCT Int. Appl., 99 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.			DATE		
					_								
WO	86070)56			A1		19861204		WO 1	985-US9	62		19850521
	W:	FI,	HU,	NO,	SU,	US							
HU	45247	7			A2		19880628		HU 1	985-302	1		19850521
HU	21033	39			В		19950328						
EP	20760)5			A1		19870107		EP 1	986-303	648		19860514
EP	P 207605		B1 19900207										
	R:	ΑT,	BE,	CH,	DE,	FR	, GB, IT,	LI,	LU,	NL, SE			
ΑT	50256	ò			Τ		19900215		AT 1	986-303	648		19860514
CA	12793	320			С		19910122		CA 1	986-509	336		19860516

IL	78831	A	19901129	IL	1986-78831		19860519
DK	8602335	A	19861122	DK	1986-2335		19860520
AU	8657580	A	19870108	AU	1986-57580		19860520
AU	560179	В2	19870402				
ES	555147	A1	19870716	ES	1986-555147		19860520
ZA	8603762	A	19880525	ZA	1986-3762		19860520
DD	261154	A5	19881019	DD	1986-290390		19860520
JP	61271287	A	19861201	JΡ	1986-117127		19860521
JP	05086953	В	19931214				
CN	86104075	A	19870311	CN	1986-104075		19860521
CN	1007248	В	19900321				
PL	147479	B1	19890630	PL	1986-259633		19860521
US	4703052	A	19871027	US	1986-10081		19861229
FI	8700219	A	19870120	FΙ	1987-219		19870120
FI	89268	В	19930531				
FI	89268	С	19930910				
NO	8700241	A	19870320	ИО	1987-241		19870120
NO	166448	В	19910415				
NO	166448	С	19910724				
SU	1556540	A3	19900407	SU	1987-4028918		19870120
AU	8775074	A	19871015	ΑU	1987-75074		19870702
AU	583991	B2	19890511				
$_{ m IL}$	83214	A	19910718	IL	1987-83214		19870716
ES	557634	A1	19880716	ES	1987-557634		19870727
ES	557634	A5	19880812				
PRIORITY	APPLN. INFO.:				1985-US962	W	19850521
				ΕP	1986-303648	А	19860514
				IL	1986-78831	Α	19860519

OTHER SOURCE(S): CASREACT 107:39794; MARPAT 107:39794

GΙ

$$R^3$$
 R^4
 (CH_2)
 R
 R^5
 R^5
 NH
 R^5
 NH
 R^5
 R^5
 NH
 NH

AB The title compds. [I; R = H; (R)2 = bond; R1 = H, pyridyl, furyl, thienyl, naphthyl, (un)substituted alkyl, cycloalkyl, Ph, etc.; R2 = H, Me; R3 = H, alkyl, PhCH2, (un)substituted Ph; R4 = H; R1R2, R2R3, R3R4 = alkylene; R5 = H, Me, Et; X = O, S, SO, SO2, etc.; n = 0-2] were prepared as hypoglycemic agents (no data). 2-HOC6H4CHO and BrCH2COPh were refluxed in DMF to give 2-benzoylbenzofuran, which was hydrogenated over Pd/C to give 2-benzyl-2,3-dihydrobenzofuran. The latter was formylated by treatment with TiCl4 and C12CHOMe in CH2Cl2 at 0-5° and the resulting 5-formyl derivative was heated at 140° with 2,4-thiazolidinedione and NaOAc to give (benzofuranylmethylene)thiazolidinedione II.

IT 109210-31-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 109210-31-3 CAPLUS

CN Benzofuran, 2-(1-methyl-1-phenylethyl)- (CA INDEX NAME)

L11 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1979:455708 CAPLUS Full-text

DOCUMENT NUMBER: 91:55708

ORIGINAL REFERENCE NO.: 91:9019a,9022a

TITLE: Carbon-13 NMR spectra of some furocoumarins AUTHOR(S): Bose, Ajay K.; Fujiwara, H.; Kamat, Vinayak S.;

Trivedi, Girish K.; Bhattacharyya, Sasanka C. CORPORATE SOURCE: Dep. Chem. Chem. Eng., Stevens Inst. Technol.,

Hoboken, NJ, USA

SOURCE: Tetrahedron (1979), 35(1), 13-16

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AB The 13C NMR spectra of the naturally occurring furocoumarins I (R = H, CMe2OH) and derivs. I (R = CHMe2, CMe2Ph, CMe2C6H4OMe-4) were studied.

IT 55710-65-1P 55710-66-2P

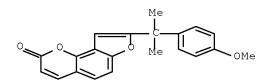
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and carbon-13 NMR of)

RN 55710-65-1 CAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-2-one, 8-(1-methyl-1-phenylethyl)- (CA INDEX NAME)

RN 55710-66-2 CAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-2-one, 8-[1-(4-methoxyphenyl)-1-methylethyl]-(CA INDEX NAME)



L11 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1975:170745 CAPLUS Full-text

DOCUMENT NUMBER: 82:170745

ORIGINAL REFERENCE NO.: 82:27281a,27284a

TITLE: Structures of two dimers formed from oroselol with

acids

AUTHOR(S): Kamat, Vinayak S.; Audichya, Thakur D.; Trivedi,

Girish K.; Bhattacharyya, Sasanka C.

CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Bombay, India SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1975), (3), 204-8

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Addnl date considered in abstracting and indexing are available from a source cited in the original document. Oroselol (I), a furocoumarin extracted from Selinium vaginatum, with acid formed dimers II and III via a carbonium ion and subsequent condensation with oroselone (IV). This mechanism was supported by the formation of V-VII from I in the presence of Lewis acids.

IT 55710-65-1P 55710-66-2P 55710-67-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 55710-65-1 CAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-2-one, 8-(1-methyl-1-phenylethyl)- (CA INDEX NAME)

RN 55710-66-2 CAPLUS

 $\texttt{CN} \qquad 2 \\ \texttt{H-Furo}[2,3-h]-1-\\ \texttt{benzopyran-2-one}, \quad 8-[1-(4-\texttt{methoxyphenyl})-1-\texttt{methylethyl}]-1-\\ \texttt{methylethyl}]-1-\\ \texttt{methylethyl}]-1-\\$

RN 55710-67-3 CAPLUS

CN 2H-Furo[2,3-h]-1-benzopyran-2-one, 8-[1-(4-ethoxyphenyl)-1-methylethyl]- (CA INDEX NAME)

=> logoff h COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 34.14 264.47

FULL ESTIMATED COST

CA SUBSCRIBER PRICE

SINCE FILE TOTAL

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

ENTRY SESSION
-4.80 -4.80

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 18:55:07 ON 07 MAR 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptansc1625

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 18:58:38 ON 07 MAR 2008 FILE 'CAPLUS' ENTERED AT 18:58:38 ON 07 MAR 2008 COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	34.14	264.47

-4.80

-4.80

CA SUBSCRIBER PRICE

=> d his

(FILE 'HOME' ENTERED AT 18:40:05 ON 07 MAR 2008)

FILE 'REGISTRY' ENTERED AT 18:40:17 ON 07 MAR 2008

L1 STRUCTURE UPLOADED

L2 3 S SSS SAM L1

L3 STRUCTURE UPLOADED

L4 0 S SSS SAM L3

L5 107 S SSS FULL L3

SAVE L5 LU10579564/A

L6 STRUCTURE UPLOADED

L7 0 S SSS L6 SAM SUB=L5

L8 38 S SSS L6 FULL SUB=L5

L9 69 S L5 NOT L8

FILE 'CAPLUS' ENTERED AT 18:53:23 ON 07 MAR 2008

L10 1 S L8 L11 5 S L9

=> activate LU10579564/A

ANSWER SET WAS CREATED IN FILE 'REGISTRY'.

An answer set can be activated only in the same file in which the search was done. Use the FILE command to switch to the correct file. Then enter ACTIVATE.

ACTIVATE QUERY ONLY? (Y)/N:y

L12 STR

L13 QUE ABB=ON PLU=ON L12

=> delete LU10579564/A

DELETE LU10579564/A? (Y)/N:y

LU10579564/A DELETED

=> save temp 15 LU10579564/A

ANSWER SET NOT SAVED.

THE ANSWER SET WAS CREATED IN FILE 'REGISTRY'.

USE THE FILE COMMAND TO CHANGE TO THE CORRECT FILE.

Answer sets must be saved in the same file in which they were created.

=> fil req

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 51.58 265.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION

CA SUBSCRIBER PRICE -4.80 -4.80

FILE 'REGISTRY' ENTERED AT 19:00:43 ON 07 MAR 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1 DICTIONARY FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> activate LU10579564/A 'LU10579564/A' NOT FOUND

The name that you entered was not found in the list of saved queries, answer sets, or L# lists for this loginid. Enter "DISPLAY SAVED" at an arrow prompt (=>) to see a list of all saved queries, answer sets, and L# lists for this loginid. To see the names of all SDI profiles, enter "DISPLAY SAVED/S". To see the names of all BATCH search requests, enter "DISPLAY SAVED/B".

=> save temp 15 LU10579564/A ANSWER SET L5 HAS BEEN SAVED AS 'LU10579564/A'

=> logoff y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	266.37
DISCOUNT ANOTHER (DOD OWN THAT IS A COOKING)	0.11100 0.110	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-4.80

STN INTERNATIONAL LOGOFF AT 19:01:21 ON 07 MAR 2008